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Blended-fuel based EDC combustion model and its application in heptane-ethanol fire simulation

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Abstract The blended-fuel based eddy-dissipation-concept combustion model was newly developed in the FireFOAM framework, and applied to simulate 30 cm×30 cm heptane-ethanol pool fire. Comparison was made of fire height, centerline temperature against experimental measurements, which shows that they match very well with each other. However, further studies are needed to examine the validation of this model in fire simulations with various scales.
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Keywords fire safety, blended-fuel based EDC combustion model, numerical simulation

Petroleum products such as heptane, gasoline, diesel, etc., are normally impure and consist of two or more components. Fuel vapour resulting from the pyrolysis of solid fuels also consists of a mixture of gas and solid components. From the standpoint of fire safety, there is hence the need to understand the fire behavior involving blended fuels and develop the predictive capability to assist related consequence analysis.

As to fire simulation, the combustion model is vital, in which the eddy dissipation concept (EDC) model has been extensively used and further focused for development. The EDC model was originally proposed by Magnussen et al.[1,2] based on energy cascading, for the computation of turbulent combustion. The original EDC formulations were successful in Reynolds averaged Navier–Stokes (RANS) applications, but in large eddy simulation (LES), there are some problems that the total kinetic energy required in the computation is not available and only the sub-grid scale (SGS) kinetic energy, which is a small part of the former, is resolved. This essentially requires the EDC model in the LES framework to be formulated with the SGS kinetic energy and eddy viscosity. Fureby et al.[3,4] directly replaced the total kinetic energy and its dissipation rate using SGS kinetic energy k_{SGS} and other SGS parameters. However, this approach is reported[3] that the predicted reaction rate is strongly dependent on grid size. The problem was thought to be caused by the direct replacement of the total kinetic energy with the SGS kinetic energy, which is much smaller than the total kinetic energy and varies with the grid resolution. Chen et al.[5] followed the energy cascade concept and derived the total kinetic energy and its dissipation rate using the SGS quantities, and developed the extended EDC model.

Following the work in Ref. 5, the authors further extended it to account for the combustion of fuels with mixed components using either infinitely fast chemistry or finite rate chemistry. For

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the present study, infinitely-fast chemistry is assumed and the fires of the heptane-ethanol blended fuels were simulated for validation against the experimental data.

Chen et al.[5] derived the total kinetic energy and its dissipation rate using the SGS quantities as $k = [3/(2C_{D1}^2)]^{1/3}(\varepsilon L')^{2/3}$, $\varepsilon = \sqrt{3/2}C_{D1}k_{SGS}^{3/2}/\Delta + (2/9)C_{D2}\upsilon k_{SGS}/\Delta^2$, where $C_{D1} = 0.5$ and $C_{D2} = 0.75$, υ and Δ are the molecular kinetic viscosity and the filter size, and k_{SGS} is obtained together with turbulence dissipation rate ε_{SGS} and turbulent viscosity ν_t by using the one-equation LES model of Menon et al.[6] The integral length scale L' is evaluated as the characteristic plume length of the fire following the wide practice of the fire research community[7] $L' = [Q/(\rho_\infty C_p T_\infty \sqrt{g})]^{2/5}$, where Q is the heat release rate (kW), ρ_∞, C_p, T_∞, and g are the ambient density, specific heat at constant pressure, temperature, and the acceleration of gravity, respectively. Thus the characteristic length L^* and velocity scale u^* of the fine structure can be written as $L^* = (2/3)(3C_{D2}^3/C_{D1}^2)^{1/4}(\upsilon^3/\varepsilon)^{1/4}$, $u^* = [C_{D2}/(3C_{D1}^2)]^{1/4}(\upsilon\varepsilon)^{1/4}$. For the present study, infinitely-fast chemistry is assumed for heptanes fire or heptane-ethanol fires as $C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$, $C_2H_6O + 3O_2 \rightarrow 2CO_2 + 3H_2O$.

The essence of the EDC is that chemical reactions take place in the fine structures. It is further assumed that the fine structures can be described as stationary homogeneous perfectly stirred reactors (PSR). Thus in each computational cell, the remaining reactants and newly formed products in the fine structure mix with the surrounding fluids through turbulent diffusion. The filtered reaction rate for the species mass-fraction transport equation can be expressed as $\bar{\omega}_i = \bar{\rho}\dot{m}^*[\gamma\chi/(1-\gamma\chi)]\left(\tilde{Y}_i - Y_i^*\right)$ where $\bar{\rho}$, γ, χ, and $\tilde{Y}_i$ are the filtered density, mass fraction of the fine structures, reacting fraction of the fine structures, and surrounding species mass fraction. The species mass fraction in fine structures Y_i^* are evaluated for the above infinitely-fast reactions as

$$Y_{f,i}^* = Y_{f,i}^{*old} - \left\{ Y_{f,i}^{*old} \Big/ \left[\sum_{j=1}^{N_F} Y_{f,j}^{*old} \Big/ \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{f,j,n} W_{f,j} \right) \right] \right\}$$
$$\min \left[\sum_{j=1}^{N_F} Y_{f,j}^{*old} \Big/ \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{f,j,n} W_{f,j} \right), Y_{O_2}^{*old} \Big/ \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{O_2,n} W_{O_2} \right) \right], \quad \text{for fuels,}$$

$$Y_{O_2}^* = Y_{O_2}^{*old} - \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{O_2,n} W_{O_2} \right)$$
$$\min \left[\sum_{j=1}^{N_F} Y_{f,j}^{*old} \Big/ \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{f,j,n} W_{f,j} \right), Y_{O_2}^{*old} \Big/ \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{O_2,n} W_{O_2} \right) \right], \quad \text{for oxidizer } O_2,$$

$$Y_{p,i}^* = Y_{p,i}^{*old} + \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{p,i,n} W_{p,i} \right) \min \left[\sum_{j=1}^{N_F} Y_{f,j}^{*old} \Big/ \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{f,j,n} W_{f,j} \right), \right.$$
$$\left. Y_{O_2}^{*old} \Big/ \text{abs}\left(\sum_{n=1}^{N_R} \upsilon'_{O_2,n} W_{O_2} \right) \right], \quad \text{for products } (CO_2 \text{ and } H_2O),$$

where N_R, N_F, υ', W_j, and Y_i^{*old} are reaction number, fuel number, stoichiometric coefficients species, molecular weight, and the species mass fraction in fine structure at last time step, respectively. The mass transfer rate between the fine structures and the surrounding fluids $\dot{m}^*$ can be calculated as $\dot{m}^* = 2u^*/L^* = (3/C_{D2})^{1/2}(\varepsilon/\upsilon)^{1/2}$. Following the work of Magnussen,[8] the mass

fraction of the fine structures might be written as $\gamma = (L^*/L')^{\alpha}$ with $\alpha = 0.2$.

Chen et al.[5] suggested that the reacting fraction of the fine structures is expressed as $\chi \approx Z/Z_{st}$ for $0 \leqslant Z < Z_{st}$ and $\chi \approx (1-Z)/(1-Z_{st})$ for $Z_{st} < Z \leqslant 1$, where Z is mixture fraction and accordingly Z_{st} denotes stoichiometric mixture fraction.

The FireFOAM code solves the spatial filtered and Favre averaged reactive Navier–Stokes equations in the LES framework. The partially stirred reactor (PASR) based soot model also developed by present authors is used for soot formation and oxidation. Since heptane-ethanol fire is normally optically-thick, the greyMeanAbsorptionEmission-based FVDOM in OpenFOAM framework is taken into account for gas and soot radiation. It should be noted that soot absorption coefficient is evaluated following the work of Chatterjee et al.,[9] $\kappa_s \approx 1\,226 f_v T$ where f_v and T are soot volume fraction and gas temperature, respectively.

The simulated heptane-ethanol pool fire has a scale of 30 cm×30 cm and the mass ratio of 0.464 9:0.535 1, corresponding to the liquid volume ratio of 1:1. The computation was set up by inputting the time-varying mass burning rate of heptane-ethanol blended fuels, as shown in Fig. 1, which was measured in experiment.

As accurate prediction of fire height and temperature is necessary for combustion model validation, the predicted flame height is first compared with the experimental measurements in Fig. 2. It should be noted that the transient fire height in experiment is characterized as the visible luminous flame height, possibly involving continuous flame region and intermittent flame region. The simulated fire height is defined by the highest location where the fuel and oxygen coexist, since infinite-rate reactions are taken into account. Figure 2 demonstrates that the predicted fire height agrees very well with the measured data at both fire growth and relatively steady stages.

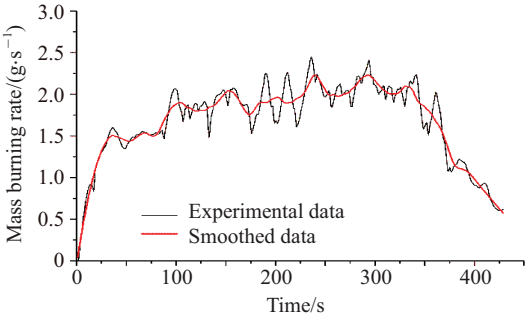

Fig. 1. Mass burning rate versus time.

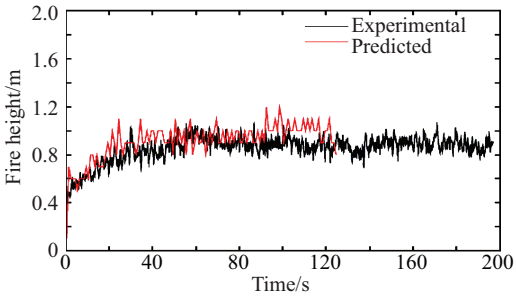

Fig. 2. Fire height versus time.

Figure 3 plots the predicted and measured temperature profiles at different centerline heights (e.g., $H = 0.2$ m, 0.6 m, 1.0 m, 1.6 m). Good agreement between the prediction and the measurement can be observed, especially when the fire falls in continuous flame regions ($H = 0.2$ m) and fire plume ($H = 1.6$ m). Near the fire base ($H = 0.2$ m), the assumption of infinitely-fast rate shows its limitation that the abruptly fast increment of fire temperature at the initial stage is different from that in the experiments. At $H = 0.6$ m and $H = 1.0$ m, the temperature is over-predicted about 200 K. This over-prediction is possibly attributed to the assumption of infinitely-fast rate. Besides, it might be also caused by fuel boiling point difference and the resultant discrepancy of heptane-ethanol mass fraction ratio between the simulation and the experiment. Furthermore, this

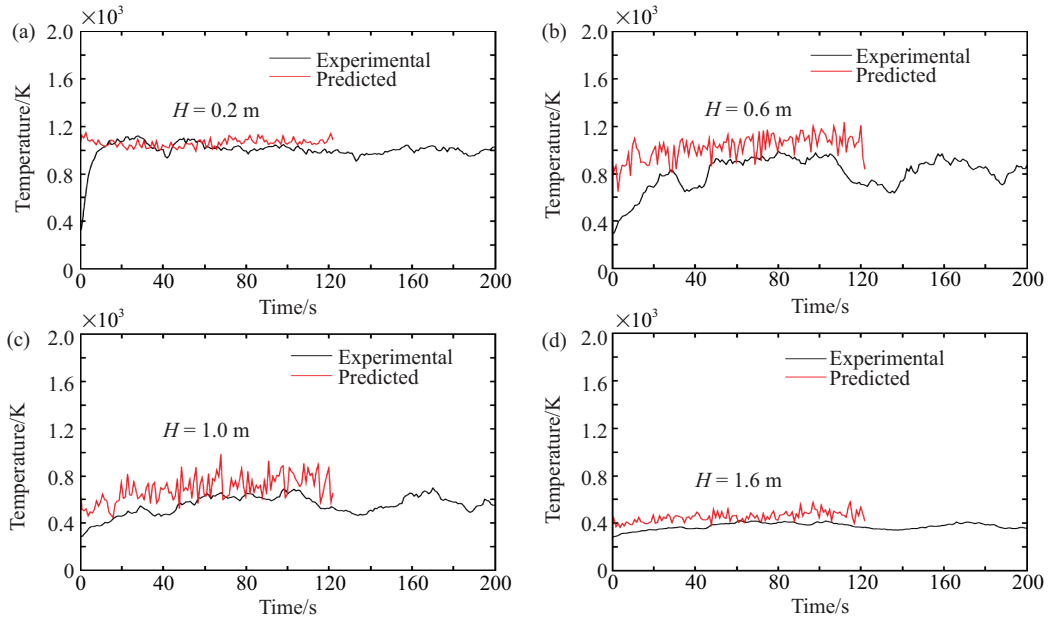

Fig. 3. Temperature versus time at different centerline heights.

discrepancy influences the change of soot formation and oxidation rates in this region, and soot endothermicity/exothermicity, etc. However, current simulation generally reproduces the experiments.

The blended-fuel based EDC combustion model was newly developed in the FireFOAM framework, and applied to simulate 30 cm×30 cm heptane-ethanol pool fire. The simulated results demonstrate good quantitative agreement with experimental measurements about fire height as well as temperature at different centerline height, which shows this model performs well in this case. However, further studies are needed to examine the validation of this model in fire simulations with various scales.

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